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# A Deterministic Method for Computer Modelling of Diffusion Effects in MRI with Application to BOLD Contrast Imaging

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## Purpose

In functional MRI using blood oxygenation level dependent (BOLD) contrast, diffusion of spins through susceptibility induced field gradients causes an increase in the MR signal for gradient echoes, and a decrease in the MR signal for spin echoes. A key step in the understanding of BOLD contrast will be in the development of good models of functional mechanisms at the capillary and small vessel level including the effects of diffusion. Computer modelling of these diffusion effects has generally been done by using random walk simulations to track the positions of a group of spins over time, and recording their phase histories(1,2). This requires the calculation of randomized trajectories for a large number of spins in order to arrive at a solution with high precision. As the physical models for structures such as capillary beds become more complex, the numbers of spins tracked must increase in order to assure uniform sampling of the space. We introduce here a method of computer modelling of these diffusion effects which uses convolution of the spin density map with a smoothing function as a means of simulating diffusion. This method is deterministic in that no random variables are used, and it is adaptable to restricted and anisotropic diffusion.

### Method

At any instant in time, the state of the spins in a voxel can be described by maps of the magnetization at subvoxel resolution. If these maps are sufficiently fine that they are smooth over a voxel, then for the purposes of the MR signal they completely define the state of the spins in that voxel, and it is not necessary to track the phase history of individual spins. In every unit of time  $\Delta t$ , the effects of diffusion and susceptibility can be described by a smoothing function and a spatially dependent phase rotation, respectively. This is the basis of the current approach. If  $\Delta t$  is small enough so that the distance spins move due to diffusion is small on the scale of the field inhomogeneities, then this will be a good approximation of the simultaneous diffusion and dephasing processes.

Beginning with a physical model for the structure to be simulated, we calculate a map of field offsets due to susceptibility gradients. At time zero uniform and coherent transverse magnetization is placed across the voxel. For each simulated time interval  $\Delta t$ , a smoothing function is applied to the magnetization map to simulate diffusion, and spatially dependent phase rotations are applied to simulate off resonance effects. For unrestricted diffusion, the smoothing function is simply convolution with a Gaussian. In addition, spatially dependent scaling of the magnetization can be applied to simulate spatially inhomogeneous T2 decay.

#### Results

The method described here was used to calculate the effect of diffusion through susceptibility induced field gradients in a simple model of a capillary bed. The model was an array of infinite cylinders whose susceptibility difference from the surrounding tissue is dependent upon the  $O_2$  saturation. The following parameters were used: blood volume=5%, capillary diameter= $7\mu m$ .  $O_2$  saturation=75%,  $\Delta \chi$ =0.076ppm for completely desaturated blood, and the capillaries were perpendicular to the main field. Using these parameters, the signal through the course of a spin echo sequence with 100ms TE was calculated and is shown in Figure 1 for various values of the diffusion coefficient. With increasing diffusion coefficient, the FID portion of the signal increases monotonically in magnitude, while the spin echo first decreases then increases in magnitude. For gradient and spin echo sequences, the calculated signal at time TE=100ms is shown in Figure 2 as as function of diffusion coefficient. The minimum for the spin echo signal occurs at a diffusion coefficient of  $0.2\mu m^2/ms$ . indicating the approximate position of the intermediate exchange regime for this geometry.

### Conclusion

The method described here provides a flexible and deterministic alternative to Monte Carlo techniques for the simulation of diffusion effects in MRI.

# Reference

- 1. Fisel C, et al. Magn. Reson. Med. 17, 336, 1991.
- Ogawa S, et al. Biophys. J. 64, 803, 1993.

